High Order Integration Schemes on the Unit Sphere

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ABSTRACT

A method for refining high order numerical integration schemes is described. Particular focus is on integration schemes over the unit sphere with octahedral symmetry. The method is powerful enough that new integration schemes can be found from rough intuitive guesses. New schemes up to order 59 are presented.

High order Gauss quadratures on a sphere are of generic interest in numerical analysis. They may have applications ranging from modeling of large scale phenomena on the globe, such as in weather forecasting, to the calculation of quantum mechanical integrals.[1-3] In a Gauss quadrature on a sphere one would expect to be able to integrate three spherical harmonics per integration point having one weight and two positional parameters. For applications, it is more convenient to use a set of integration points with symmetry so that a much reduced parameter set needs to be dealt with. Because of the peculiarities of the triangulation of a sphere, the expectation just mentioned is usually not exactly fulfilled. Lower order schemes sometimes overperform or underperform quite significantly. An example of overperformance is the 72-point scheme with icosahedral symmetry of order 15.[4] It integrates 256 functions, significantly more than the 216 expected. Integration schemes with octahedral symmetry, as pioneered by Lebedev,[5,6,10] are somewhat easier to handle, and often a subset of integration points can be used that is compatible with the symmetry-unique wedge. Low order octahedral schemes tend slightly to underperform in efficiency, but, for high order the expected efficiency is closely approached. Therefore, the focus of this article is on schemes with octahedral symmetry.

The basic idea for the refinement of integration schemes is independent of symmetry. Consider the function set of spherical harmonics $Y_{\ell,m}$ up to some order ℓ_{max}. The property of a Gauss integration scheme, defined by a set of points $\hat{r}_i$ on the unit sphere and weights w_i with $i = 1 \ldots n$, can be seen as the solution of the nonlinear set of equations in $\hat{r}_i$ and w_i

$$\sum_{i=1}^{n} Y_{\ell,m}(\hat{r}_i)w_i - \frac{1}{\sqrt{4\pi}}\delta_{\ell,0} = 0 \qquad (1)$$

Here, $\delta_{\ell,0}$ is the Kronecker delta, allowing for the fact that $Y_{0,0}$ has a nonvanishing integral over the sphere. Sufficiently near a solution, refinements can be made using a multidimensional Newton

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algorithm. This will be shown in further detail for the case with symmetry.

If a symmetric integration scheme is used, most of the equations (1) are automatically fulfilled. In the case of octahedral symmetry it is useful to observe that the set of $K(l_{max})$ functions

$$\{Y_{\ell,m}\}, \quad \ell = 4n_4 + 6n_6 < \ell_{max}, \quad m = 4(n_4 + n_6), \quad n_4, n_6 = 0, 1, 2, 3 \ldots$$

contains all polynomials with full octahedral symmetry up to order ℓ_{max}; compare also Ref. 6. The $Y_{\ell,m}$ values are the usual real spherical harmonics and can be generated conveniently by recursion relations. (The non-fully symmetric polynomials admixed to the $Y_{\ell,m}$ of the set are projected out in integrations over the whole sphere.) The author finds that the norm of the $Y_{\ell,m}$ helps to control accuracy for the integrals of high order functions. Table I illustrates the function set for the case of $\ell = 17$.

The entire set of integration points is built-up from subsets of special points of octahedral symmetry, each having one or more free parameters:

TABLE I.
$Y_{\ell,m}$ Set for $\ell = 17$.

k	n_4	n_6	ℓ	m
1	0	0	0	0
2	1	0	4	4
3	0	1	6	4
4	2	0	8	8
5	1	1	10	8
6	3	0	12	12
7	0	2	12	8
8	2	1	14	12
9	4	0	16	16
10	1	2	16	12

The set "6" of 6 points, the vertices of the octahedron, contributes one parameter, the weight. Also, the sets "8," the vertices of the cube and the set "12," the 12 points related to $(\sqrt{2}/2, \sqrt{2}/2, 0)$ contribute one weight parameter each. The sets of type "24a," the 24 points related to $(u, u, \sqrt{1 - 2u^2})$ and "24b," $(v, 0, \sqrt{1 - v^2})$ contribute one weight and one positional parameter u and v, respectively. Finally, the sets "48," the 48 general points related to $(r, s, \sqrt{1 - r^2 - s^2})$, contribute one weight and two positional parameters r and s.

TABLE II.
Points and Weights for Gaussian Integrations over the Unit Sphere.

Order **17** Type 1 1 0 3 1 0 with 110 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0038 2827 0494 9371 616
.5773 5026 9189 62576	.5773 5026 9189 62576	.0097 9373 7512 4875 125
.1851 1563 5344 73617	.1851 1563 5344 73617	.0082 1173 7283 1911 110
.3956 8947 3055 94191	.3956 8947 3055 94191	.0095 9547 1336 0709 628
.6904 2104 8382 29218	.2159 5729 1845 84883	.0099 4281 4891 1781 033
.4783 6902 8812 15020	.0000 0000 0000 00000	.0096 9499 6361 6630 283

Order **23** Type 1 1 1 4 1 1 with 194 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0017 8234 0447 2446 112
.5773 5026 9189 62576	.5773 5026 9189 62576	.0055 7338 3178 8487 380
.7071 0678 1186 54752	.0000 0000 0000 00000	.0057 1690 5949 9771 019
.4446 9331 7871 74373	.4446 9331 7871 74373	.0055 1877 1467 2736 137
.2892 4656 2757 54386	.2892 4656 2757 54386	.0051 5823 7711 8053 831
.6712 9734 4269 52263	.3141 9699 4182 58608	.0056 0870 4082 5879 968
.1299 3354 4765 00669	.1299 3354 4765 00669	.0041 0677 7028 1693 941
.3457 7021 9761 12827	.0000 0000 0000 00000	.0050 5184 6064 6148 085
.5251 1857 2443 64202	.1590 4171 0538 35295	.0055 3024 8916 2330 937

Order **29** Type 1 1 0 6 2 2 with 302 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0008 5459 1172 5128 148
.5773 5026 9189 62576	.5773 5026 9189 62576	.0035 9911 9285 0255 715
.7011 7664 1608 95449	.1292 3867 2710 51493	.0036 5004 5807 6772 554
.6566 3294 1021 96118	.3710 3417 8384 82119	.0036 0482 2601 4198 817
.4729 0541 3258 10046	.4729 0541 3258 10046	.0035 7672 9661 7433 671
.3515 6403 4557 01051	.3515 6403 4557 01051	.0034 4978 8424 3058 833
.2219 6452 3629 41784	.2219 6452 3629 41784	.0031 0895 3122 4136 753
.0961 8308 5226 14784	.0961 8308 5226 14784	.0023 5210 1413 6891 644
.5718 9558 9187 89607	.0000 0000 0000 00000	.0036 0082 0932 2164 603
.2644 1528 8706 06625	.0000 0000 0000 00000	.0029 8234 4963 1718 039
.5448 6773 7258 07738	.2510 0347 5177 04651	.0035 7154 0554 2733 871
.4127 7240 8316 85310	.1233 5485 3258 33274	.0033 9231 2205 0061 702

TABLE II.
(continued)

Order **35** Type 1 1 1 7 2 4 with 434 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0005 2658 9796 8224 436
.5773 5026 9189 62576	.5773 5026 9189 62576	.0025 1231 7418 9273 072
.7071 0678 1186 54752	.0000 0000 0000 00000	.0025 4821 9972 0026 072
.6909 3463 0750 91106	.2126 4682 4707 55207	.0025 3040 3801 1863 550
.6456 6647 0742 42561	.4077 1266 4897 76951	.0025 1326 7174 5975 644
.4914 3426 3778 47465	.4914 3426 3778 47465	.0025 0172 5168 4029 361
.3927 2597 6336 80022	.3927 2597 6336 80022	.0024 4537 3437 3129 800
.2861 2890 1030 76384	.2861 2890 1030 76384	.0023 0269 4782 2274 158
.1774 8360 5460 91578	.1774 8360 5460 91578	.0020 1427 9020 9185 282
.0756 8084 3671 78018	.0756 8084 3671 78018	.0014 6249 5621 5946 138
.2102 7252 2857 30696	.0000 0000 0000 00000	.0019 1095 1282 1795 323
.4715 9869 1151 31592	.0000 0000 0000 00000	.0024 1744 2375 6389 808
.3344 3631 4534 34549	.0992 1769 6364 29237	.0022 3660 7760 4378 487
.4502 3303 8258 26254	.2054 8236 9640 30437	.0024 1693 0044 3247 753
.5550 1523 6107 68072	.3104 2840 3516 65415	.0024 9664 4054 5530 860
.5905 1570 4892 52711	.1068 0182 6075 80483	.0025 1223 6854 5634 951

Order **41** Type 1 1 0 8 4 6 with 590 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0001 0090 0575 3378 758
.5773 5026 9189 62576	.5773 5026 9189 62576	.0018 5140 1687 3890 461
.7040 4760 4331 46996	.0929 1900 5968 83211	.0018 6862 1951 8306 975
.6808 4561 9880 24238	.2699 9719 2170 17240	.0018 6486 9634 5606 001
.6372 3669 1594 18917	.4334 2680 7860 54810	.0018 4976 4397 5168 892
.5044 7558 0609 26046	.5044 7558 0609 26046	.0018 4502 7774 0822 388
.4217 5447 3343 98773	.4217 5447 3343 98773	.0018 1641 7498 8262 214
.3320 1962 0867 29379	.3320 1962 0867 29379	.0017 4494 6469 0023 229
.2391 7494 3365 56047	.2391 7494 3365 56047	.0016 2780 1612 6848 035
.1402 4070 7389 35403	.1402 4070 7389 35403	.0015 5768 2751 9901 693
.0916 1634 3286 05240	.0000 0000 0000 00000	.0012 6809 6888 6048 433
.2032 6292 5184 19433	.0000 0000 0000 00000	.0011 1839 6541 4769 017
.3936 4042 3729 78295	.0000 0000 0000 00000	.0017 2870 3512 0530 033
.6126 2355 8129 29648	.0000 0000 0000 00000	.0018 5519 0562 9473 527
.2811 4771 6234 28322	.0895 9875 9118 93791	.0014 6973 5312 3693 616
.3817 5470 9085 81117	.1732 7600 2384 98666	.0016 8196 5191 4742 022
.4745 2376 4789 86998	.2642 2260 6562 45780	.0017 8763 7287 6796 954
.5612 7905 0759 20534	.3518 9965 8738 35832	.0018 4007 3568 5528 423
.5032 4791 9969 64975	.0888 6791 0181 86295	.0018 0725 3681 7113 700
.5976 8324 3207 48616	.1815 4345 6435 17542	.0018 5272 8973 9424 312

Order **47** Type 1 1 1 9 4 9 with 770 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0011 6853 3560 8691 628
.5773 5026 9189 62576	.5773 5026 9189 62576	.0014 1212 1593 0643 264
.7071 0678 1186 54752	.0000 0000 0000 00000	.0014 4686 4595 0992 776
.1144 1365 1233 36336	.1144 1365 1233 36336	.0010 4784 1886 4629 224
.1994 4675 7085 48970	.1994 4675 7085 48970	.0012 3925 4758 4848 484
.2840 1278 3682 59530	.2840 1278 3682 59530	.0013 2592 9579 2415 379
.3664 6411 4165 48296	.3664 6411 4165 48296	.0013 7560 9775 8625 958
.4435 6118 0525 13995	.4435 6118 0525 13995	.0013 9993 4886 3558 624
.5143 5709 5753 33968	.5143 5709 5753 33968	.0014 0962 2121 8822 673
.6305 2081 1966 71812	.4526 4446 4622 79973	.0014 1087 4649 9638 577
.6716 4784 3372 93865	.3126 9529 7350 24947	.0014 1348 8763 9034 478
.6981 2332 0101 74177	.1588 9512 2204 05632	.0014 3669 4668 5816 802
.1204 7667 9312 64991	.0000 0000 0000 00000	.0010 9015 4357 4180 667
.3094 0302 3154 80606	.0000 0000 0000 00000	.0001 8691 3784 4803 852
.3488 4276 4301 83016	.0000 0000 0000 00000	.0011 2842 6765 2336 505
.5322 4214 2854 17946	.0000 0000 0000 00000	.0013 8445 5802 6568 455
.2324 9923 4092 67532	.0661 6159 9334 37003	.0011 8539 2388 5095 502
.3247 7344 4096 82044	.1456 8618 7651 36356	.0012 9490 2166 4637 693
.4105 6989 0393 49425	.2283 2839 1321 27622	.0013 5258 5742 0363 760
.4921 3658 0851 14203	.3071 4431 9015 43855	.0013 9250 2590 8786 082
.5654 8849 8125 88755	.3827 1180 6250 74657	.0014 0732 5789 4372 725
.4371 3473 6939 46563	.0797 0715 1879 39190	.0013 1289 5430 7755 017
.5232 0749 4731 97761	.1589 2620 2398 64833	.0013 7846 3289 8490 457
.6028 3033 9943 86521	.2366 7220 2538 73893	.0014 1254 5060 9821 936
.6203 7164 7217 42807	.0798 2328 8260 30880	.0014 2898 3531 4095 131

Order **53** Type 1 1 0 12 4 12 with 974 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0001 4382 9419 0527 431
.5773 5026 9189 62576	.5773 5026 9189 62576	.0011 2577 2288 2870 041
.0429 2963 5453 41347	.0429 2963 5453 41347	.0004 9480 2934 1949 241
.1051 4268 5408 64042	.1051 4268 5408 64042	.0007 3579 9010 9125 470
.1750 0248 6762 30874	.1750 0248 6762 30874	.0008 8891 3277 1304 384
.2477 6533 7965 02568	.2477 6533 7965 02568	.0009 8883 4783 8921 435
.3206 5671 2395 59574	.3206 5671 2395 59574	.0010 5329 9681 7094 706
.3916 5207 4984 99835	.3916 5207 4984 99835	.0010 9277 8807 0145 785
.4590 8258 7418 76237	.4590 8258 7418 76237	.0011 1438 9394 0632 272
.5214 5638 8841 58605	.5214 5638 8841 58605	.0011 2372 4788 0515 553
.6253 1702 4465 41989	.4668 5890 5695 74328	.0011 2523 9325 2438 136
.6637 9267 4452 31699	.3446 1365 4237 43822	.0011 2615 3271 8159 050
.6910 4103 9849 83007	.2119 5415 1850 18465	.0011 3028 6931 1238 408
.7052 9070 0745 77603	.0716 2440 1449 95566	.0011 3498 6534 3639 549
.1236 6867 6265 79899	.0000 0000 0000 00000	.0006 8233 6792 7109 931
.2940 7771 1446 83870	.0000 0000 0000 00000	.0009 4541 5816 0447 096
.4697 7538 4920 76491	.0000 0000 0000 00000	.0010 7442 9975 3856 791
.6334 5632 4113 95669	.0000 0000 0000 00000	.0011 2930 0086 5691 317
.2029 1287 5277 75228	.0597 4048 6141 81342	.0008 4368 8450 0901 954
.4602 6219 4248 40539	.1375 7604 0847 36365	.0010 7525 5720 4488 846
.5030 6739 9966 20357	.3391 0165 2633 62857	.0011 0857 7236 8644 620
.2817 6064 2244 21343	.1271 6751 9143 98195	.0009 5664 7532 3783 357
.4331 5612 9172 01574	.2693 1207 4041 35125	.0010 8066 3250 7173 907
.6256 1673 5858 08142	.1419 7864 5260 19183	.0011 2679 7131 1962 946
.3798 3952 1685 91567	.0670 9284 6007 38255	.0010 2256 8715 3580 612
.5517 5054 2142 35205	.0705 7738 1832 56172	.0011 0896 0267 7131 075
.6029 6191 5615 91869	.2783 8884 7788 21546	.0011 2279 0653 4357 658
.3589 6063 2958 90958	.1979 5789 3891 74069	.0010 3240 1847 1174 598
.5348 6664 3813 54765	.2087 3070 6110 32740	.0011 0724 9382 2838 539
.5674 9975 4607 43735	.4055 1221 3787 28359	.0011 2178 0048 5199 721

Order **59** Type 1 1 1 13 4 16 with 1202 points.

X	Y	Weight
.0000 0000 0000 00000	.0000 0000 0000 00000	.0001 1051 8923 3267 572
.5773 5026 9189 62576	.5773 5026 9189 62576	.0009 1331 5978 6443 561
.7071 0678 1186 54752	.0000 0000 0000 00000	.0009 2052 3273 8090 741
.0371 2636 4496 57089	.0371 2636 4496 57089	.0003 6904 2189 8017 899
.0914 0060 4122 62223	.0914 0060 4122 62223	.0005 6039 9092 8680 660
.1531 0778 5246 99062	.1531 0778 5246 99062	.0006 8652 9762 9282 609
.2180 9288 9166 06116	.2180 9288 9166 06116	.0007 7203 3855 1145 630
.2839 8745 3220 01746	.2839 8745 3220 01746	.0008 3015 4595 8894 795
.3491 1776 0096 37644	.3491 1776 0096 37644	.0008 6866 9255 0179 628
.4121 4314 6144 43092	.4121 4314 6144 43092	.0008 9270 7628 5846 890
.4718 9936 2714 91266	.4718 9936 2714 91266	.0009 0608 2023 8568 219
.5273 1454 5284 23366	.5273 1454 5284 23366	.0009 1197 7725 4940 867
.6209 4753 3244 40192	.4783 8093 8076 95216	.0009 1287 2013 8604 181
.6569 7227 1185 72905	.3698 3086 6459 42597	.0009 1307 1493 5691 735
.6841 7883 0907 01434	.2525 8395 5700 71777	.0009 1528 7378 4554 116
.7012 6043 3012 36308	.1283 2618 6659 72300	.0009 1874 3627 4321 654
.1072 3822 1547 81661	.0000 0000 0000 00000	.0005 1769 7731 2965 694
.2582 0689 5949 69680	.0000 0000 0000 00000	.0007 3311 4368 2101 417
.4172 7529 5530 67168	.0000 0000 0000 00000	.0008 4632 3283 6379 928
.5700 3669 1179 25033	.0000 0000 0000 00000	.0009 0311 2269 4253 992
.1771 7740 2261 53253	.0521 0639 4770 11284	.0006 4857 7845 3163 257
.2475 7164 6342 62876	.1115 6409 5715 64867	.0007 4350 3091 0982 369
.3173 6152 4661 19767	.1746 5516 7757 86261	.0008 1017 3149 7468 018
.3854 2911 5066 92237	.2390 2784 7938 17240	.0008 5562 9925 7311 812
.4507 4225 9315 70644	.3029 4669 7352 89819	.0008 8502 8234 1265 444
.5123 5184 8641 98708	.3649 8322 6059 76536	.0009 0226 9293 8426 915
.5693 7024 9846 84411	.4238 6447 8152 23403	.0009 1057 6025 8970 126
.3354 6162 8906 64885	.0590 5888 8532 35508	.0007 9985 2789 1839 054
.4090 2684 2708 53572	.1217 2350 5109 59870	.0008 4833 8957 4594 331
.4785 3206 7592 24352	.1857 5051 9454 73351	.0008 8110 4818 2425 720
.5434 3035 6969 39004	.2494 1121 6236 22365	.0009 0100 9167 7105 086
.6031 1616 9309 63100	.3112 2759 4714 96082	.0009 1078 1357 9482 705
.4932 2211 8485 12846	.0626 6250 6241 54169	.0008 8032 0867 9738 260
.5632 1230 2076 20997	.1267 7748 0068 42827	.0009 0213 4229 9040 653
.6269 8055 0902 43917	.1906 0182 2277 92370	.0009 1315 7800 3189 435
.6394 2796 3474 91023	.0642 4549 2242 20589	.0009 1580 1617 4693 465

The type specification indicates the number of occurrences for the subsets of points with 6, 8, 12, 24_a, 24_b and 48 points. Each subset is specified by one line in the table. The full set of points is $(\pm x, \pm y, \pm z)$ and permutations; with $z = \sqrt{1 - x^2 - y^2}$.

It is useful to consider both positional and weight parameters as elements p_j of a parameter vector $\mathbf{p}$. Integration schemes can be constructed by providing a number of parameters exactly matching the number of nontrivial equations $K(\ell_{max})$. Efficient schemes can be constructed by using, as much as possible, the lower sets. Lebedev[6] has given a table specifying the number of sets for schemes up to $\ell_{max} = 51$. To refine a cubic symmetric integration scheme, it is useful to define a set of residuals, R_k, which depends on the full parameter set, $\mathbf{p}$

$$\sum_{i=1}^{n} Y_{\ell(k),m(k)}(r_i(\mathbf{p}))w_i(\mathbf{p}) - \frac{1}{\sqrt{4\pi}}\delta_{\ell(k),0} = R_k(\mathbf{p}), \quad k = 1 \ldots K(\ell_{max}) \qquad (2)$$

Here n is the total number of integration points. For a sufficiently accurate estimate of $\mathbf{p}$ an improved estimate $p_j^+ = p_j + q_j$ can be obtained by solving the set of linear equations

$$\sum_{j=1}^{K} \frac{\partial R_k}{\partial p_j} q_j = -R_k \qquad (3)$$

Equations (2) and (3) form a multidimensional Newton method and are iterated to convengence. The fast final rate of convergence of the Newton method helps to reach the simultaneous vanishing of all R_k to an accuracy limited only by roundoff error. The final residuals are $|R_k| \approx \sqrt{n/4\pi}\,\epsilon$ with $\epsilon = 2^{-55} \approx 3.e - 17$ for VAX VMS and $\epsilon = 2^{-52} \approx 2.e - 16$ for IBM RISC. It is useful to scale-down the q_j in the initial iterations such that a reasonable maximum correction is never exceeded in order to suppress chaotic trajectories in parameter space.

This scheme was applied to find integration schemes of order 35 and 41[8,9] with 434 and 596 points and, in this work, of order 41, 47, 53, and 59 with 590, 770, 974, and 1202 points, respectively.

Final refinements of the parameter values were carried out in "quadruple precision" so that the accuracy of all 17 decimals presented here can be guaranteed. Since the integration points are on the unit sphere, the redundant column for the z-component $z = \sqrt{1 - x^2 - y^2}$ has been omitted. The type specification indicates how many times the point sets 6, 8, 12, 24a, 24b, and 48 were used.

The scheme of order 35 has appeared in print before.[10,11] The group[11] has "brute-force-optimized" the Lebedev grid to arrive at an accuracy of $5.e - 12$ for the integration of the worst function. Lebedev has given, in a series of publications,[5-7,12] 12 decimal tabulations for order up to $l = 53$.

A type specification for the scheme of order 41 and 47 has been proposed in ref. 6 and used in Ref. 12. Here, schemes of order 41 and 47 with a modified type specification are given in the tables. Refinements of the schemes of order 41 and 47 given in Ref. 12 were, however, also successful. Since lower order schemes are obviously used more frequently than higher ones, 17 decimal values for a selection of Lebedev schemes are also presented in Table II.

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References

1. DMol Version 1.0 1988, Biosym Inc., San Diego, CA.
2. B. Delley, *J. Chem. Phys.*, **92**, 508 (1990).
3. A. Becke, *J. Chem. Phys.*, **88**, 2547 (1988).
4. A. H. Stroud, *Approximate Calculation of Multiple Integrals*, Prentice Hall, Englewood Cliffs, 1971.
5. V. I. Lebedev, *Zh. Vychisl. Mat. Mat. Fiz.*, **15**, 48 (1975).
6. V. I. Lebedev, *Zh. Vychisl. Mat. Mat. Fiz.*, **16**, 293 (1976).
7. V. I. Lebedev, *Sibirsk. Mat. Zh.*, **18**, 132 (1977).
8. DMol Version 2.0 1989, Biosym Inc., San Diego, CA.
9. B. Delley (unpublished data), 1989.
10. V. I. Lebedev, Theory of cubature formulas and numerical mathematics. In Proceedings of the Conference on Differential Equations in Numerical Mathematics, S. Sobolev, Ed., Nauka, Novosibirsk 1980, p. 110.
11. O. Treutler and R. Ahlrichs, *J. Chem. Phys.*, **102**, 346 (1995).
12. V. I. Lebedev and A. L. Skorokhodov, *Russ. Acad. Sci. Dokl. Math.*, **45**, 587 (1992).